CH5350: Applied Time-Series Analysis

Random Variables and Moments: Review

Arun K. Tangirala

Department of Chemical Engineering, IIT Madras

Arun K. Tangirala, IIT Madras Applied Time-Series Analysis 1

Random Variable

Informal definition

A **random variable** (RV) is one whose value set contains at least two elements, i.e., it draws one value from at least two possibilities. The space of possible values is known as the **outcome space or sample space**.

Formal definition (Priestley, 1981)

A random variable X is a mapping from the sample space $\mathbb S$ onto the real line s.t. to each element $s \subset \mathbb S$ there corresponds a unique real number.

Focus of this course: Continuous-valued random variables

Distribution and Density functions

Probability distribution function

Also known as the **cumulative distribution function**: $F(x) = \Pr(X \le x)$

$$F(x) = \Pr(X \le x)$$

When the density function exists, i.e., for continuous-valued RVs,

Density functions

1 Area yields probability
$$\left| \Pr(a < x < b) = \int_a^b f(x) \, dx \right| \implies \int_{-\infty}^\infty f(x) \, dx = 1$$

2 Derivative of c.d.f.: $f(x) = \frac{dF(x)}{dx}$

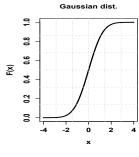
$$f(x) = \frac{dF(x)}{dx}$$

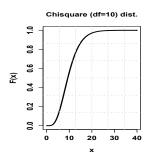
Arun K. Tangirala, IIT Madras

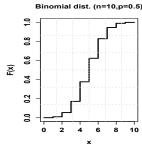
Applied Time-Series Analysis

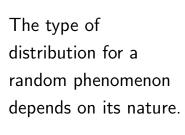
3

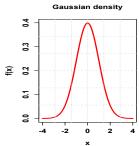
Examples: c.d.f. and p.d.f.

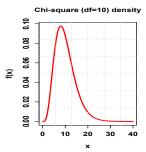


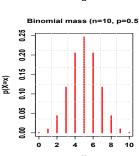












Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

Practical Aspects: Moments of a p.d.f.

- ▶ It may not be necessary to know the p.d.f. in practice!
- ▶ What is of interest in practice is (i) the most likely value and/or the expected outcome (mean) and (ii) how far the outcomes are spread (variance). These are related to what are known as moments of the density function.

The n^{th} moment of a p.d.f. is defined as

$$M_n(X) = \int_{-\infty}^{\infty} x^n f(x) \, dx$$
 (1)

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

5

Linear random process and moments

It turns out that for linear processes, predictions of random signals and estimation of model parameters it is sufficient to have the knowledge of **mean**, **variance** and **covariance** (for the multivariate case), *i.e.*, it is sufficient to know the first and second-order moments of p.d.f.

Mean and Variance: Important moments!

Mean

Mean, a.k.a. the expectation of the RV, is defined as

$$E(X) = \mu_X = \int_{-\infty}^{\infty} x f(x) \, dx \tag{2}$$

Variance

The variance of a RV measures the average spread of outcomes around its mean,

$$\sigma_X^2 = E((X - \mu_X)^2) = \int_{-\infty}^{\infty} (x - \mu_X)^2 f(x) \, dx \tag{3}$$

Note: Integration in (2) and (3) are across the outcome space and NOT across time.

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

7

Remarks

► Prediction perspective:

The mean is the best prediction \hat{X} of the RV X in the minimum mean square error sense, *i.e.*,

$$\mu = \arg \left[\min_{c} E(X - \hat{X})^2 \text{ s.t. } \hat{X} = c \right]$$

ightharpoonup Applying the **expectation operator** E to a RV or its function produces its "average" or expected value.

$$E(g(X)) = \int_{-\infty}^{\infty} g(x)f(x) dx$$
 (4)

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

8

Points to note

▶ As (3) suggests, σ_X^2 is the **second central moment** of f(x). Further,

$$\sigma_X^2 = E(X^2) - \mu_X^2 \tag{5}$$

- ► The variance definition is in the space of outcomes. It should not be confused with the widely used variance definition for a series or a signal (sample variance).
- Large variance indicates far spread of outcomes around its statistical center. Naturally, in the limit as $\sigma_X^2 \to 0$, X becomes a **deterministic** variable.

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

c

BIVARIATE / MULTIVARIATE ANALYSIS

Joint density

Where bivariate analysis is concerned, we start to think of **joint probability density functions**.

Consider two continuous-valued RVs X and Y. The probability that these variables take on values in a rectangular cell is given by the **joint density**

$$Pr(x_1 \le x \le x_2, y_1 \le y \le y_2) = \int_{y_1}^{y_2} \int_{x_1}^{x_2} f(x, y) \, dx \, dy$$

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

11

Marginal and conditional p.d.f.s

Associated with this joint probability (density function), we can ask two questions:

- What is the probability $\Pr(x_1 \leq X \leq x_2)$ regardless of the outcome of Y and vice versa? (marginal density)
- What is the probability $\Pr(x_1 \le X \le x_2)$ given Y has occurred and taken on a value Y = y? (conditional density)
 - \blacktriangleright Strictly speaking, one cannot talk of Y taking on an exact value, but only of values within an infinitesimal neighbourhood of y.

Marginal and Conditional densities

Marginal density

The marginal density of a RV X (Y) with respect to another RV Y (X) is given by

$$f_X(x) = \int_{-\infty}^{\infty} f(x, y) dy$$
 likewise, $f_Y(y) = \int_{-\infty}^{\infty} f(x, y) dx$ (6)

Conditional density

The conditional density of Y given X = x (strictly, between x and x + dx) is

$$f_{Y|X=x}(y) = \frac{f(x,y)}{f(x)} \tag{7}$$

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

13

Conditional Expectation and Prediction

In several situations we are interested in "predicting" the outcome of one phenomenon given the outcome of another phenomenon.

Conditional expectation

The conditional expectation of Y given X=x is

$$E(Y|X=x) = \int_{-\infty}^{\infty} y f_{Y|X=x}(y) \, dy = \phi(x)$$
(8)

The conditional expectation is the best predictor of Y given X among all the predictors that minimize the mean square prediction error

Independence

(Frequentist school)

Two random variables are said to be independent if and only if

$$f(x,y) = f_X(x)f_Y(y)$$
(9)

Alternatively (Bayesian school)

Two random variables are said to be independent if and only if

$$f_Y(y|x) = f_Y(y)$$
 or $f_X(x|y) = f_X(x)$ (10)

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

15

Covariance

The statistic that measures the **co-variation** of two RVs is given by the second-order moment of the joint p.d.f.:

$$\sigma_{XY} = E((X - \mu_X)(Y - \mu_Y)) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} (x - \mu_X)(y - \mu_Y) f(x, y) \, dx \, dy$$
 (11)

$$= E(XY) - E(X)E(Y) \tag{12}$$

It is useful to collect the variations and co-variation in a single **variance-covariance** matrix

$$\Sigma_X = \begin{bmatrix} \sigma_{X_1}^2 & \sigma_{X_1 X_2} \\ \sigma_{X_2 X_1} & \sigma_{X_2}^2 \end{bmatrix}$$

Covariance for vector quantities

In the general scenario, for a vector of random variables,

$$\mathbf{X} = \begin{bmatrix} X_1 & X_2 & \cdots & X_N \end{bmatrix}^T$$

we work with the variance-covariance matrix

$$\Sigma_{\mathbf{X}} = E((\mathbf{X} - \mu_{\mathbf{X}})(\mathbf{X} - \mu_{\mathbf{X}})^{T}) = \begin{bmatrix} \sigma_{X_{1}}^{2} & \sigma_{X_{1}X_{2}} & \cdots & \sigma_{X_{1}X_{N}} \\ \sigma_{X_{2}X_{1}} & \sigma_{X_{2}}^{2} & \cdots & \sigma_{X_{2}X_{N}} \\ \vdots & \ddots & \ddots & \vdots \\ \sigma_{X_{N}X_{1}} & \sigma_{X_{N}X_{2}} & \cdots & \sigma_{X_{N}}^{2} \end{bmatrix}$$

Arun K. Tangirala, IIT Madras Applied Time-Series Analysis 17

Properties of the covariance matrix

- It is a **symmetric** measure: $\sigma_{XY} = \sigma_{YX}$, i.e., it is not a directional measure. Consequently it cannot be used to sense causality (cause-effect relation).
- ▶ The covariance matrix $\Sigma_{\mathbf{X}}$ is a **symmetric, positive semi-definite** matrix $\Longrightarrow \lambda_i(\Sigma_{\mathbf{X}}) > 0 \ \forall i$
- ► Most importantly, covariance is only a measure of linear relationship between two RVs, i.e.,

When $\sigma_{XY} = \sigma_{YX} = 0$, there is no linear relationship between X and Y

lacktriangle Linear transformation of the random variables ${f Z}={f A}{f X}$ results in

$$\Sigma_{\mathbf{Z}} = E((\mathbf{Z} - \mu_{\mathbf{Z}})(\mathbf{Z} - \mu_{\mathbf{Z}})^{T}) = \mathbf{A}\Sigma_{\mathbf{X}}\mathbf{A}^{T}$$
(13)

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

18

Correlation

To overcome the unbounded and scaling-sensitivity issues, a normalized version of covariance known as **correlation** is introduced:

$$\rho_{XY} = \frac{\sigma_{XY}}{\sigma_X \sigma_Y} \tag{14}$$

- ▶ The correlation defined above is also known as Pearson's correlation
- ► Other forms of correlations exist, namely, reflection correlation coefficient,

 Spearman's rank correlation coefficient, Kendall's tau rank correlation coefficient

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

19

Unity correlation

Boundedness

For all bivariate distributions with finite second order moments,

$$|\rho_{XY}| \le 1 \tag{15}$$

with equality if, with probability 1, there is a linear relationship between X and Y.

Correlation measures linear dependence. Specifically,

- i. $|\rho_{XY}|=1\Longleftrightarrow Y=\alpha X+\beta$ (Y and X are linearly related with or without an intercept)
- ii. $\rho_{XY}=0 \Longleftrightarrow X$ and Y have no linear relationship (non-linear relationship cannot be detected)

Uncorrelated variables

Two RVs are said to be **uncorrelated** if $\sigma_{XY} = 0 \Longrightarrow \rho_{XY} = 0$. This also implies,

$$E(XY) = E(X)E(Y)$$
 (16)

- ▶ Uncorrelatedness \iff NO **linear** relationship between X and Y.
- ▶ $|\rho_{XY}| < 1$ if and only if $Y = \alpha X + \varepsilon$, where ε is another RV due to other effects (e.g., noise, non-linearities). In fact, (assuming $\sigma_{\varepsilon X} = 0$),

$$\rho_{YX} = \pm \frac{1}{\sqrt{1 + \frac{\sigma_{\epsilon}^2}{\alpha^2 \sigma_X^2}}} \le \pm 1$$

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

21

Independence vs. Uncorrelated variables

Independence \Longrightarrow Uncorrelated condition but NOT vice versa.

Thus independence is a stronger condition.

If the variables X and Y have a bivariate Gaussian distribution, Independence \iff Uncorrelated condition.

Therefore, in all such cases, independence and lack of correlation are equivalent.

Connections b/w Correlation and Linear regression

Correlation between two RVs is naturally related to the linear regression problem.

Given two (zero-mean) RVs X and Y, consider two related linear regression (prediction) problems.

$$\hat{Y} = bX \qquad \qquad \hat{X} = \tilde{b}Y \tag{17}$$

Denote the optimal estimates that minimize $E(\varepsilon^2)=E(Y-\hat{Y})^2$ and $E(\varepsilon^2)=E(X-\hat{X})^2$ as b^* and \tilde{b}^* , respectively. Then,

$$\boxed{\rho_{XY}^2 = b^* \tilde{b}^*} \qquad \qquad \text{Note:} \quad b^* = \frac{\sigma_{XY}}{\sigma_X^2}; \quad \tilde{b}^* = \frac{\sigma_{XY}}{\sigma_Y^2}$$
(18)

Zero correlation implies no linear fit in either direction.

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

23

Remarks, limitations, ...

- ► Correlation is only a mathematical / statistical measure. It does not take into account any physics of the process that relates X to Y.
- lacktriangle High values of correlation only means that a linear model can be fit between X and Y. It does not mean that in reality there exists a linear process that relates X to Y
- ▶ Correlation is symmetric, i.e., $\rho_{XY} = \rho_{YX}$. Therefore, it is not a cause-effect measure, meaning it cannot detect direction of relationships
- ► Correlation is primarily used to determine if a linear model can explain the relationship:

Remarks, limitations, ...

...contd.

- ► High values of **estimated** correlation may imply linear relationship over the experimental conditions, but a non-linear relationship over a wider range.
- ▶ Absence of correlation only implies that no linear model can be fit. Even if the true relationship is linear, noise can be high, thus limiting the ability of correlation to detect linearity
- ▶ Correlation measures only linear dependencies. Zero correlation means E(XY) = E(X)E(Y). In contrast, independence implies f(x,y) = f(x)f(y)

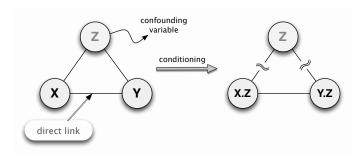
Despite its limitations, correlation and its variants remain one of the most widely used measures in data analysis

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

25

Resolving confounding: Conditional (partial) correlation



▶ If the **conditional correlation** vanishes, then the connection is purely indirect, else there exists a direct relation

Correlation measures total (linear) connectivity, whereas conditional or partial version measures "direct" association.

Partial covariance

The conditional or partial covariance is defined as

$$\sigma_{XY.Z} = \text{cov}(\epsilon_{X.Z}, \epsilon_{Y.Z})$$
 where $\epsilon_{X.Z} = X - \hat{X}^{\star}(Z), \ \epsilon_{Y.Z} = Y - \hat{Y}^{\star}(Z)$

where $\hat{X}^{\star}(Z)$ and $\hat{Y}^{\star}(Z)$ are the **optimal predictions** of X and Y using Z.

Partial correlation (PC)

$$\rho_{XY.Z} = \frac{\sigma_{XY.Z}}{\sigma_{\epsilon_{X.Z}}\sigma_{\epsilon_{Y.Z}}} = \frac{\rho_{XY} - \rho_{XZ}\rho_{ZY}}{\sqrt{(1 - \rho_{XZ}^2)}\sqrt{(1 - \rho_{ZY}^2)}}$$
(19)

▶ Partial correlation ≡ Analysis in the inverse domain.

Arun K. Tangirala, IIT Madras Applied Time-Series Analysis 27

Partial correlation: Example

Consider two RVs X=2Z+3W and Y=Z+V where V, W and Z are zero-mean RVs. Further, it is known that i.e., $\sigma_{VW}=0=\sigma_{VZ}=\sigma_{WZ}$.

Evaluating the covariance between X and Y yields

$$\sigma_{YX} = E((2Z + 3W)(Z + V)) = 2E(Z^2) = 2\sigma_Z^2 \neq 0$$

implying X and Y are correlated. However, applying (19), it is easy (with a bit of effort) to see that

$$\rho_{YX.Z} = 0$$

Thus, X and Y are not correlated given Z.

Partial correlation by inversion

Partial correlation coefficients can also be computed from the inverse of **covariance** (or **correlation**) matrix as follows.

Assume we have M RVs X_1, X_2, \cdots, X_M . Let $\mathbf{X} = \begin{bmatrix} X_1 & X_2 & \cdots & X_M \end{bmatrix}^T$.

- Construct the covariance (or correlation) matrix $\Sigma_{\mathbf{X}}$ (or $\Omega_{\mathbf{X}}$).
- Determine the inverse of covariance (or correlation) matrix, $\mathbf{S}_{\mathbf{X}} = \Sigma_{\mathbf{X}}^{-1}$ (or $\mathbf{P}_{\mathbf{X}} = \Omega_{\mathbf{X}}^{-1}$).
- **3** The partial correlation between X_i and X_j conditioned on all $\mathbf{X} \setminus \{X_i, X_j\}$ is then:

$$\rho_{X_i X_j, \mathbf{X} \setminus \{X_i, X_j\}} = -\frac{s_{ij}}{\sqrt{s_{ii}} \sqrt{s_{jj}}} = -\frac{p_{ij}}{\sqrt{p_{ii}} \sqrt{p_{jj}}}$$
(20)

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

29

Partial correlation and Linear regression

Partial correlation enjoys a relation with the regression models as does correlation.

Consider three random variables X_1, X_2, X_3 . To understand the PC between X_1 and X_2 conditioned on X_3 , construct the "forward" and "reverse" linear predictors:

$$\hat{X}_1 = b_{12}X_2 + b_{13}X_3, \qquad \qquad \hat{X}_2 = b_{21}X_1 + b_{23}X_3 \tag{21}$$

Then, we have an interesting result:

The squared-PC between X_1 and X_2 is the product of optimal coefficients

$$\boxed{\rho_{12.3}^2 = b_{12}^{\star} b_{21}^{\star}}, \quad b_{12}^{\star} = \frac{\sigma_1}{\sigma_2} \left(\frac{\rho_{12} - \rho_{13} \rho_{23}}{1 - \rho_{23}^2} \right), \quad b_{21}^{\star} = \frac{\sigma_2}{\sigma_1} \left(\frac{\rho_{12} - \rho_{13} \rho_{23}}{1 - \rho_{13}^2} \right) \tag{22}$$

where the [.]* denotes optimal (MMSE) estimates.

Uses of partial correlation

- ▶ In time-series analysis, partial correlations are used in devising what are known as partial auto-correlation functions, which are used in determining the order of auto-regressive models
- ► The partial cross-correlation function and its frequency-domain counterpart, known as partial coherency function, find good use in time-delay estimation
- ▶ In model-based control applications, partial correlations are used in quantifying the impact of model-plant mismatch in model-predictive control applications.

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

31

Semi-partial correlation: Discounting selectively

Semi-partial correlation

It examines the correlation between X_1 and **residualized** X_2 (w.r.t. X_3)

$$\rho_{1(2.3)} = \frac{\rho_{12} - \rho_{13}\rho_{23}}{\sqrt{1 - \rho_{23}^2}}$$

- "Closer" to regression coefficient than the partial correlation (why?)
- ► Smaller in value than the partial correlation coefficient (why?)

Commands in R

Commands	Utility
mean, var, sd	sample mean, variance and standard deviation
colMeans,rowMeans	means of columns and rows
median, mad	sample median and median absolute deviation
cov,corr,cov2cor	covariance, correlation and covariance-to-correlation
lm, summary	linear regression and summary of fit

Arun K. Tangirala, IIT Madras Applied Time-Series Analysis 33

Computing partial correlation in R

Use the ppcor package (due to Seongho Kim)

▶ pcor: Computes partial correlation for each pair of variables given others.

Syntax: pcormat <- pcor(X)</pre>

where ${\bf X}$ is a matrix with variables in columns. The default is Pearson correlation, but it can also compute Kendall and Spearman (partial) correlations. Result is given in pcormatsestimate

Computing semi-partial correlation in R

Use the ppcor package (due to Seongho Kim)

spcor: Computes semi-partial correlation

```
Syntax: spcormat <- spcor(X)</pre>
```

The semi-partial correlation between X and Y given Z is computed as the correlation between X and Y.Z, i.e., only Y is conditioned on Z. The matrix of semi-partial correlations is asymmetric

Arun K. Tangirala, IIT Madras

Applied Time-Series Analysis

35

Sample usage

```
1 w <- rnorm(200); v <- rnorm(200); z <- rnorm(200); # ...
    Generate w,v and z
2 x <- 2*z + 3*w; y = z+ v; # Generate x and y
3 cor(cbind(x,y)) # Compute correlation matrix between x ...
    and y
4 pcor(cbind(x,y,z)))$estimate # Compute partial correlation ...
    matrix</pre>
```